

Formfactors in the half-filled Hubbard model

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We consider dynamical spin-spin correlation functions in the one dimensional repulsive half-filled Hubbard model. We propose an exact expression for the two spinon formfactor of spin operators. We use this to derive the two spinon contribution to the dynamical structure factor.

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I. INTRODUCTION

The calculation of dynamical correlation functions is one of the main challenges in low dimensional theories of statistical and condensed matter physics. The large distance behaviour (corresponding to very low energies) can be effectively extracted for critical theories by using bosonization or Bethe Ansatz and conformal field theory techniques [1–4]. The results obtained in this way for models like the Heisenberg XXZ chain have been successfully applied to neutron scattering experiments of quasi-1D magnetic insulators, see e.g. [5,6]. However, from an experimental point of view not only very low energies are of interest. In magnetic materials described by the spin-1/2 Heisenberg model [5,6] the scattering continuum is measured up to energies of twice the exchange, which is outside the realm of reliability of the above methods. It therefore would be useful to have a method for the calculation of (Fourier transforms of) correlation functions at all energy scales. Another setting that is outside the realm of the above methods are systems with a spectral gap, see e.g. [6–9]. Some systems with spectral gap can be dealt with by the *formfactor* approach to quantum correlation functions [10–13,9]. The advantage of this method is that it is in principle not constrained to very low energies. The formfactor approach can also be implemented for critical systems, in particular this has been done for the Heisenberg XXX chain [14,15]. The results are useful for the analysis of the observed two-spinon scattering continuum in magnetic insulators like KCuF₃. In the present paper we consider the problem of calculating formfactors in the one dimensional half-filled Hubbard model. In a way this model is the “parent” of the Heisenberg model used for the description of the aforementioned magnetic insulators: the charge sector is gapped and the spin sector for large repulsion between electrons is described by an effective Heisenberg Hamiltonian. However, if the system is probed at energy scales of

the order of the Coulomb repulsion e.g. by photoemission experiments, which measure the single-particle spectral function, the itinerant nature of the system emerges and it is necessary to calculate correlation functions in the half-filled Hubbard chain in order to describe the experiments. In the present context it is of particular interest to calculate formfactors of the electronic creation and annihilation operators, as these results could be directly applied to the ARPES data of [16]. The easier problem of determining formfactors of the spin operators in the Hubbard model is the subject of the present work.

We consider the repulsive half filled Hubbard model [17]. The Hamiltonian is ($U > 0$)

$$H(U) = - \sum_{j=1}^L \sum_{\sigma=\uparrow,\downarrow} \left(c_{j,\sigma}^\dagger c_{j+1,\sigma} + c_{j+1,\sigma}^\dagger c_{j,\sigma} \right) + 4U \sum_{j=1}^L \left(n_{j,\uparrow} - \frac{1}{2} \right) \left(n_{j,\downarrow} - \frac{1}{2} \right). \quad (1)$$

This Hamiltonian exhibits an $SO(4)$ symmetry [18], i.e. it commutes with the generators

$$S = \sum_{j=1}^L c_{j,\uparrow}^\dagger c_{j,\downarrow}, \quad S^z = \sum_{j=1}^L \frac{1}{2} (n_{j,\downarrow} - n_{j,\uparrow}), \quad (2)$$

$$\eta = \sum_{j=1}^L (-1)^j c_{j,\uparrow} c_{j,\downarrow}, \quad \eta^z = \frac{1}{2} \sum_{j=1}^L (n_{j,\uparrow} + n_{j,\downarrow} - 1). \quad (3)$$

The complete spectrum of low-lying excitations was determined in [19]. It consists of pairs of scattering states of four elementary excitations, which form the fundamental representation of $SU(2) \times SU(2)$. There is a doublet of uncharged, gapless spin-1/2 particles called spinons. Their energy and momentum (as functions of the rapidity variable β) are given by [20,19]

$$p_s(\beta) = \frac{\pi}{2} - \int_0^\infty \frac{d\omega}{\omega} \frac{J_0(\omega) \sin(\omega 2U\beta/\pi)}{\cosh(\omega U)}, \quad \varepsilon_s(\beta) = 2 \int_0^\infty \frac{d\omega}{\omega} \frac{J_1(\omega) \cos(\omega 2U\beta/\pi)}{\cosh(\omega U)}, \quad (4)$$

where $J_{0,1}$ are Bessel functions. The other two elementary excitations carry charge $\pm e$ but no spin. They are called holon and antiholon and have a gap proportional to U . Their energy and momentum are

$$\begin{aligned}\varepsilon_c(k) &= 2U + 2 \cos k + 2 \int_0^\infty \frac{d\omega}{\omega} \frac{J_1(\omega) \cos(\omega \sin k) e^{-\omega U}}{\cosh(\omega U)} \\ p_c(k) &= \pi/2 - k - \int_0^\infty \frac{d\omega}{\omega} \frac{J_0(\omega) \sin(\omega \sin k) e^{-\omega U}}{\cosh(\omega U)}.\end{aligned}\quad (5)$$

II. DYNAMICAL STRUCTURE FACTOR

In this paper we consider the dynamical structure factor, which is the Fourier transform of the dynamical spin-spin correlation function and which is measured by inelastic neutron scattering. The formfactor expansion is given by

$$\begin{aligned}S(\omega, p) &= \int_{-\infty}^{\infty} dt \sum_{m=-\infty}^{\infty} e^{i\omega t + ipm} \langle 0 | \sigma_m^+(t) \sigma_0^-(0) | 0 \rangle \\ &= \sum_{n=2}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} dt \sum_{m=-\infty}^{\infty} e^{i\omega t + ipm} \prod_{k=1}^n \left(\int_{-\infty}^{\infty} \frac{d\beta_k}{2\pi} \right) \\ &\quad \times \langle 0 | \sigma_m^+(t) | \beta_n \dots \beta_1 \rangle_{\varepsilon_n \dots \varepsilon_1} \langle \beta_1 \dots \beta_n | \sigma_0^-(0) | 0 \rangle \\ &= \sum_{n=2}^{\infty} S_n(\omega, p),\end{aligned}\quad (6)$$

where the labels ε_j enumerate the four possible elementary excitations. Our notation is the following: $\varepsilon = \pm$ denotes a spinon with spin up/down, $\varepsilon = 1, -1$ denotes an antiholon/holon. As excitations involving holons and antiholons have gaps the main contribution to the correlation function (6) comes from multi-spinon excitations. By virtue of related results obtained in other gapless models [21] we expect that the main contribution is due to excitations involving only two spinons. Because of the spin- $SU(2)$ symmetry the 2-spinon contribution is of the form

$$\begin{aligned}S_2(\omega, p) &= 2\pi \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\beta_1}{2\pi} \int_{-\infty}^{\infty} \frac{d\beta_2}{2\pi} \\ &\quad \times \exp(im[p + p_s(\beta_1) + p_s(\beta_2)]) \\ &\quad \times \delta(\omega - \varepsilon_s(\beta_1) - \varepsilon_s(\beta_2)) \left| \langle 0 | \sigma_1^+ | \beta_2 \beta_1 \rangle_{--} \right|^2.\end{aligned}\quad (7)$$

We propose the following expression for the two-spinon formfactor

$$\begin{aligned}f(\beta_1, \beta_2)_{--} &= \langle 0 | \sigma_1^+ | \beta_2 \beta_1 \rangle_{--} = \\ &= c A_-(\beta_2 - \beta_1) / [\sinh(i\pi/4 - \beta_1/2) \sinh(i\pi/4 - \beta_2/2)], \\ A_-(\beta) &= \exp \left(- \int_0^\infty \frac{dt}{t} \frac{\sinh^2(t[1 - \beta/i\pi]) \exp(t)}{\sinh(2t) \cosh(t)} \right).\end{aligned}\quad (8)$$

Here c is the usual common constant factor in all formfactors. We presently cannot determine its exact numerical value although it is possible to obtain an estimate by considering various sum rules. Let us now provide some evidence for the validity of (8).

For integrable relativistic quantum field theories one generically has a formfactor expansion of the form (6), (7) for correlation functions of local operators. The formfactors themselves are determined by the following set of axioms [10,11]

Axiom 1. The form factors have the symmetry property

$$\begin{aligned}f(\dots, \beta_i, \beta_{i+1}, \dots)_{\varepsilon_1, \dots, \varepsilon_i, \varepsilon_{i+1}, \dots, \varepsilon_n} S_{\varepsilon_i, \varepsilon_{i+1}}^{\varepsilon'_i, \varepsilon'_{i+1}}(\beta_i - \beta_{i+1}) \\ = f(\dots, \beta_{i+1}, \beta_i, \dots)_{\varepsilon_1, \dots, \varepsilon'_{i+1}, \varepsilon'_i, \dots, \varepsilon_n}\end{aligned}\quad (9)$$

Axiom 2. The formfactors fulfil the tensor-valued Riemann-Hilbert problem

$$f(\beta_1 \dots \beta_n + 2\pi i)_{\varepsilon_1 \dots \varepsilon_n} = f(\beta_n \beta_1 \dots \beta_{n-1})_{\varepsilon_n \varepsilon_1, \dots, \varepsilon_{n-1}} \quad (10)$$

Axiom 3. In the absence of bound states the only singularities of $f(\beta_1, \dots, \beta_n)_{\varepsilon_1, \dots, \varepsilon_n}$ for $n \geq 3$ are at the points $\beta_i = \beta_j + \pi i$, $i > j$. These singularities are first order poles (annihilation poles) with residues

$$\begin{aligned}i \operatorname{Res}_{\beta_n = \beta_{n-1} + \pi i} f(\beta_1 \dots \beta_n)_{\varepsilon_1, \dots, \varepsilon_n} = \\ f(\beta_1, \dots, \beta_{n-2})_{\varepsilon'_1, \dots, \varepsilon'_{n-2}} \delta_{\varepsilon_n, -\varepsilon_{n-1}} \left(\delta_{\varepsilon_1}^{\varepsilon'_1} \dots \delta_{\varepsilon_{n-2}}^{\varepsilon'_{n-2}} - \right. \\ \left. S_{\tau_1, \varepsilon_1}^{\varepsilon'_{n-1}, \varepsilon'_1}(\beta_{n-1} - \beta_1) \dots S_{\varepsilon_{n-1}, \varepsilon_{n-2}}^{\tau_{n-3}, \varepsilon'_{n-2}}(\beta_{n-1} - \beta_{n-2}) \right).\end{aligned}\quad (11)$$

Here $S_{\gamma\delta}^{\alpha\beta}(\beta)$ is the 2-particle scattering matrix of the theory under consideration. Although these axioms are based on crossing symmetry and relativistic energy-momentum relations, there is evidence that the axioms hold true even for formfactors of certain nonrelativistic lattice models. In particular, it was shown by Pakuliak [22] that the known formfactors [14] of the XXZ Heisenberg lattice model fulfil Axioms 1-3. We believe that this will be true for integrable models of statistical mechanics and condensed matter physics as long as the ground state is a singlet under the action of an infinite dimensional symmetry algebra like a Yangian or $U_q(\widehat{sl(2)})$. In particular, the formfactor (8) can be seen to fulfil Axioms 1-3

$$\begin{aligned}f(\beta_1, \beta_2 + 2\pi i)_{--} &= f(\beta_2, \beta_1)_{--}, \\ f(\beta_1, \beta_2)_{--} &= S_{--}(\beta_2 - \beta_1) f(\beta_2, \beta_1)_{--},\end{aligned}\quad (12)$$

where $S_{--}(\beta)$ is the dressed S-matrix for scattering of spinons in the spin triplet state with $S^z = -1$

$$S_{--}(\beta) = \frac{\Gamma(-\beta/2\pi i) \Gamma(1/2 + \beta/2\pi i)}{\Gamma(\beta/2\pi i) \Gamma(1/2 - \beta/2\pi i)}.\quad (13)$$

We think that the fact that (8) fulfils (12) is a good indication for the correctness of the “minimal formfactor” $A_-(\beta)$. The full result (8) can be checked exactly in the limit $U \rightarrow \infty$, where the half-filled Hubbard model (1) reduces to the isotropic spin-1/2 Heisenberg chain

$$H_{XXX} = J \sum_{j=1}^L \vec{S}_j \cdot \vec{S}_{j+1} , \quad (14)$$

where the exchange is given by $J = 1/U$. The spinon formfactors for this model have been calculated in [14,15]. The dynamical structure factor can be represented in the form (6), where the sum is over all spinon states. The 2-spinon contribution is [15]

$$\begin{aligned} S_2^{XXX}(\omega, p) &= 2\pi \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\beta_1}{2\pi} \int_{-\infty}^{\infty} \frac{d\beta_2}{2\pi} \\ &\times \exp(im[p + p(\beta_1) + p(\beta_2)]) \\ &\times \delta(\omega - \varepsilon(\beta_1) - \varepsilon(\beta_2)) \left| \langle 0 | \sigma_1^+ | \beta_2 \beta_1 \rangle_{--} \right|^2 \end{aligned} \quad (15)$$

where

$$\begin{aligned} \langle 0 | \sigma_1^+ | \beta_2 \beta_1 \rangle_{--} &= c' A_-(\beta_2 - \beta_1) \\ &\times (\sinh(i\pi/4 - \beta_1/2) \sinh(i\pi/4 - \beta_2/2))^{-1} \end{aligned} \quad (16)$$

Here the dressed energy $\varepsilon(\beta)$ and momentum $p(\beta)$ are given by

$$\varepsilon(\beta) = J\pi/2 \cosh \beta , \quad p(\beta) = \operatorname{arccot}(\sinh \beta) . \quad (17)$$

It is a straightforward to see that in the limit $U \rightarrow \infty$ $S_2(\omega, p)$ indeed reduces to $S_2^{XXX}(\omega, p)$. The $U \rightarrow \infty$ limit of $\varepsilon_s(\beta)$ and $p_s(\beta)$ is derived for example in [25]. We believe that (8) is correct for any value of $U > 0$. In [23] an independent derivation for formfactors of σ^+ in the isotropic Heisenberg XXX chain (14) was given by using representation theory of a central extension of a double of the $sl(2)$ -Yangian. For this purpose σ^+ can be represented as the density of one of the zeroth level Yangian generators (E_0 in the notation of [24]). Because the spin part of the Yangian [24] of the Hubbard model is the same as in the XXX case, we believe that the XXX result can be “lifted” to the half-filled Hubbard model in the way presented above.

In order to perform the integrals over $\beta_{1,2}$ in (7) we need to discuss some properties of the continuum of two-spinon excited states. Energy and momentum are given by

$$\begin{aligned} E(\beta_1, \beta_2) &= \varepsilon_s(\beta_1) + \varepsilon_s(\beta_2) , \\ P(\beta_1, \beta_2) &= p_s(\beta_1) + p_s(\beta_2) \bmod 2\pi , \end{aligned} \quad (18)$$

where $\beta_{1,2} \in (-\infty, \infty)$. The upper boundary is obtained by taking $\beta_1 = \beta_2$ and the lower one by taking $\beta_1 = \pm\infty$. We denote the respective dispersion relations by $\omega_{U,L}(p)$. In Fig.1 we plot the 2-spinon continuum for $U = 5$.

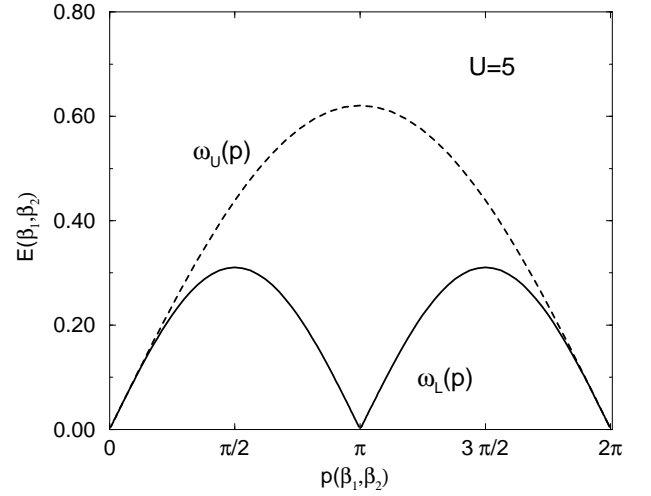


FIG. 1. Continuum of two spinon excitations for $U = 5$.

In the first Brillouin zone there is a unique solution $(\bar{\beta}_1, \bar{\beta}_2)$ to the set of equations

$$\begin{aligned} \omega &= \varepsilon_s(\beta_1) + \varepsilon_s(\beta_2) , \\ p &= p_s(\beta_1) + p_s(\beta_2) , \end{aligned} \quad (19)$$

as long as ω is chosen within the interval $(\omega_L(p), \omega_U(p))$. This allows us to take the integrals over $\beta_{1,2}$ in (7) with the result

$$\begin{aligned} S_2(\omega, p) &= \bar{c} \Theta(\omega - \omega_L(p)) \Theta(\omega_U(p) - \omega) |A_-(\bar{\beta}_2 - \bar{\beta}_1)|^2 \\ &\times (\cosh(\bar{\beta}_1/2) \cosh(\bar{\beta}_2/2))^{-1} \\ &\times \left| \frac{\partial \varepsilon_s(\bar{\beta}_1)}{\partial \bar{\beta}_1} \frac{\partial p_s(\bar{\beta}_2)}{\partial \bar{\beta}_2} - (1 \leftrightarrow 2) \right|^{-1} , \end{aligned} \quad (20)$$

where $\Theta(x)$ is the Heaviside function. Due to the complicated relation between energy/momentum and the spectral parameter β we have not been able to simplify (20) further. It is however in a form that can be readily analyzed numerically. Let us first discuss constant momentum scans, i.e. the behaviour of $S(\omega, p)$ as a function of ω for fixed p . At the antiferromagnetic wave vector $p = \pi$ the singularity at zero frequency is

$$\begin{aligned} S(\omega, \pi) &\propto \frac{1}{\omega} \sqrt{\log \frac{1}{\omega}} \text{ for } \omega \rightarrow 0 , \\ S(\omega, \pi) &\propto \sqrt{\omega_U(\pi) - \omega} \text{ for } \omega \rightarrow \omega_U(\pi) . \end{aligned} \quad (21)$$

The power-law behaviour in the $\omega \rightarrow 0$ limit agrees with the result obtained from finite-size corrections and conformal field theory [1]. In Fig.2 we plot $S_2(\omega, \pi)$ on a logarithmic scale. One can see that the $\frac{1}{\omega} \sqrt{\log \frac{1}{\omega}}$ behaviour holds even for relatively large values of ω .

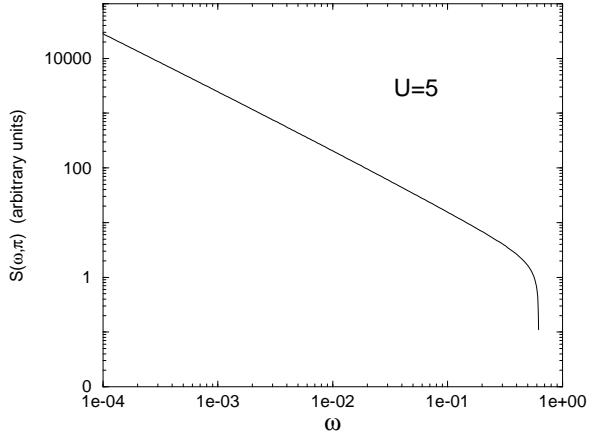


FIG. 2. Constant momentum scan for $p = \pi$ and $U = 5$.

In Fig.3 we plot $S_2(0.3, p)$ as a function of the momentum p . Obviously the dynamical structure factor is nonzero only if intermediate states with energy $\omega = 0.3$ and momentum p are available i.e. inside the dispersion of the 2-spinon continuum shown in Fig.1.

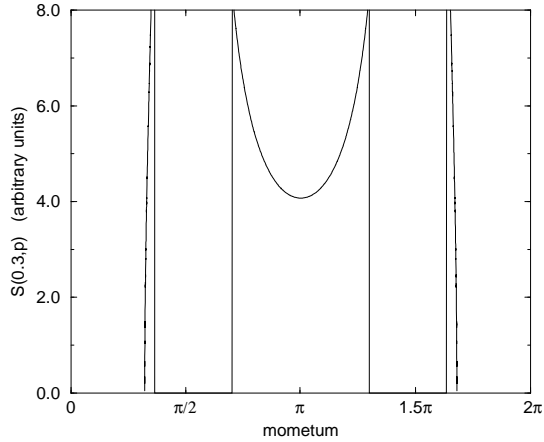


FIG. 3. Constant energy scan for $\omega = 0.3$ and $U = 5$.

Finally, let us discuss consequences of our results for the attractive Hubbard model. It is known that the half-filled repulsive Hubbard model can be mapped to the half-filled attractive Hubbard model by means of the unitary transformation defined by

$$\mathcal{U}c_{j,\downarrow}\mathcal{U}^\dagger = c_{j,\downarrow}, \quad \mathcal{U}c_{j,\uparrow}\mathcal{U}^\dagger = (-1)^j c_{j,\uparrow}^\dagger, \quad (22)$$

under which $H(U)$ goes to $H(-U)$ and the spin (2) and eta-pairing operators (3) get interchanged. The repulsive ground state is mapped into the attractive one [26], which in turn implies that the two spinon states considered above get mapped into the charge-wave states

discussed in [19] (which have up to a shift in momentum by π the same dispersion as the two spinon states). As a consequence we can obtain from (8) the two charge-wave contribution to pairing and density-density correlation functions in the attractive half-filled Hubbard model

$$\begin{aligned} &\langle 0 | c_{m,\uparrow}^\dagger(t) c_{m,\downarrow}^\dagger(t) c_{0,\downarrow}(0) c_{0,\uparrow}(0) | 0 \rangle, \\ &\langle 0 | n_m(t) n_0(0) | 0 \rangle, \end{aligned} \quad (23)$$

where $n_m = c_{m,\uparrow}^\dagger c_{m,\uparrow} + c_{m,\downarrow}^\dagger c_{m,\downarrow}$. The analysis of the corresponding Fourier transforms is identical to the one carried out above for the dynamical structure factor.

III. CONCLUSIONS

We have proposed an exact expression for the two spinon formfactor of spin operators in the half-filled Hubbard chain. We explicitly calculated the corresponding contribution to the dynamical structure factor. Our proposal (8) can be extended to multispinon formfactors of spin operators [27]. We think that very recent developments [28] in the calculation of formfactors in integrable lattice models will make it possible to prove (8) rigourously and also lead to the determination of formfactors of the fermion operators in the near future.

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